

1,1,2,2-Tetrafluoro-2-(1,1,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
104729-49-9 | DTXSID40446988

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.04

Global applicability domain: Outside

Local applicability domain index: 2.63e-01

Confidence level: 8.26e-01

Nearest Neighbors from the Training Set

Image not found

1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 2.51

Predicted: 2.40

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Triallyl phosphate

Measured: 1.20

Predicted: 1.41

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o-Toluenesulfonamide

Measured: 2.57

Predicted: 2.00

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Fenthion sulfone

Measured: 3.24

Predicted: 1.71

Image not found

Triethyl phosphate

Measured: 1.29

Predicted: 1.38